Model Based Reactor Optimization for a Heterogeneously Catalyzed Fast Highly Endothermal Reaction

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Introduction

Process intensification and optimization of industrial plants in the chemical process industries is key for the implementation of more energy efficient processes with reduced carbon dioxide emissions at increased productivity. For this purpose, the design and optimization of the reactor as central process unit must aim at achieving optimal reaction conditions along the reaction route. In this regard, the multi-level reactor design (MLRD) methodology (Freund et al., 2019, Peschel et al., 2010) has proven to be a suitable approach and therefore is applied in this study on the example of an extremely fast highly endothermal reaction. The aim was to optimize the existing industrial process to achieve a higher space-time-yield with a more energy efficient reactor concept, thereby also reducing the carbon dioxide footprint.

In catalytic tubular reactors, suitable reaction conditions along the reactor axis can be realized by different options. One promising approach is the use of novel catalyst supports, and particularly of so-called Periodic Open Cellular Structures (POCS) as introduced by Freund and Schwieger (Inayat et al., 2011). To maximize catalyst inventory in the reactor, a combination of POCS with catalyst pellets in the void space, known as packed POCS (Ambrosetti et al., 2020), is investigated in this study. The bottleneck of this exemplary reaction is the heat transfer into the catalyst bed. The high endothermicity of the reaction can result in cold spots in the bed, leading to a decrease in reaction rate and thereby to a lower productivity. Therefore, the goal is to determine a method to increase the heat transport into the catalyst bed and define optimal reaction conditions to achieve a high space-time-yield.

Intrinsic Reaction Kinetics Measurements

In the first step of the MLRD methodology, the optimal reaction conditions for the exemplary reaction are determined using the intrinsic reaction kinetics in the optimization. To handle the challenges in kinetic measurements for extremely fast highly endothermal reactions, high weight hourly space velocities (WHSV) are necessary to ensure measurements in the kinetic regime, unbiased from external mass or heat transfer limitations. For this purpose, a dedicated lab plant setup with a Berty-type reactor, which exhibits approximately ideal behavior at high volume flows inside the reactor, was designed and built. The composition of the product stream was analyzed with a micro gas chromatograph, allowing for a high precision analysis at relatively high temporal resolution. With this dedicated experimental setup, extensive kinetic measurements over a wide range of reaction conditions were performed. Afterwards, parameter estimation for the reaction kinetic model was carried out, resulting in an intrinsic reaction kinetics model.

Optimization with Packed POCS

The high thermal conductivity of the continuous structure of POCS improves the heat transport compared to conventional randomly packed beds and results in a more homogeneous temperature distribution along the reactor axis (Ambrosetti et al., 2020). Therefore, a reactor model containing correlations describing the heat transport within the packed POCS as well as the pressure drop along the reactor was implemented. The simulated concentration and temperature profiles along the reactor were compared to the results of the reactor model of the industrial reactor, which serves as a reference case. A following optimization study was performed using the reactor model of the tubular reactor with packed POCS.

Conclusions

The MLRD approach resulted in a reactor design for approaching the optimal reaction conditions. Inserting packed POCS into the tubular reactor leads to an enhanced heat transfer compared to a conventional randomly packed bed. This results in a decrease of the temperature drop at the cold spot and to a higher temperature level at the reactor outlet. Consequently, a higher overall conversion is reached, thereby increasing the productivity and the energy efficiency of the process.

References

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